Topological aspects of chaotic scattering in higher dimensions

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Abstract

We investigate the topological properties of invariant sets associated with the dynamics of scattering systems with three or more degrees of freedom. We show that the asymptotic separation of one degree of freedom from the rest in the asymptotic regime, a common property in a large class of scattering models, defines a dynamical object with phase space separating invariant manifolds and an invariant set with larger dimension than that of the set defined by bounded orbits. In particular, the set of typical periodic orbits involving all the degrees of freedom of the system form a nowhere dense subset of the large invariant set.

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I. INTRODUCTION

Chaotic scattering in open Hamiltonian systems with two degrees of freedom has become a well understood phenomenon [1]. A central role is played in these processes by the *chaotic invariant set* which consists of all the bounded orbits, i.e. those without the simple incoming and outgoing asymptotic motions characteristic of the system. The invariant set is globally hyperbolic which means that its orbits can attract incoming trajectories along their stable manifolds extending smoothly towards the asymptotic region. The trajectories are then forced into a temporarily chaotic behaviour in the vicinity of the chaotic invariant set, before eventually escaping along the unstable manifold of the set. For initial conditions exactly on a stable manifold branch, the trajectories may even become asymptotically trapped by the corresponding bounded orbit; this leads to singularities on a fractal set in the scattering functions.

In the two-dimensional Poincaré sections generally used for the representation of the dynamics, bounded orbits appear as points forming a double Cantor set structure. Stable and unstable manifolds of the bounded orbits show up as continuous lines. The stable manifold lines are of codimension one in these cases, so they can separate the phase space into distinct regions corresponding to qualitatively different scattering trajectories. The same property makes it also possible to capture the singularities associated with the irregular nature of scattering in any generic one-dimensional family of initial conditions.

There are two traditional ways to look at the chaotic invariant set [1]. (i) One is to consider a simple periodic orbit that plays a basic role in organizing the scattering process: usually this periodic orbit lies at the edge of the scattering region, and trajectories approaching it escape or do not escape the interaction region depending on which side of its stable manifold they are while approaching. We will call such objects *gates* in the following [2,3]; as we will show, they can be more complicated than periodic orbits. The set of all the homoclinic points (intersections of the stable and unstable manifolds) consists of trajectories doubly asymptotic to the gate. The chaotic invariant set is then obtained as the closure (in a mathematical sense) of the set of the intersection points and contains also *all* the possible periodic orbits of the system. (ii) The alternative approach considers the chaotic invariant set as the closure of the set of all the periodic orbits; the closure in this case generates trajectories doubly asymptotic to periodic ones. These two ways give equivalent results in systems with two degrees of freedom (apart from pathological exceptions), and many studies have made use of this duality in the analysis of such chaotic scattering processes.

In fact, it has become an article of faith that all chaotic invariant sets, whether related to transient or permanent chaos, can be considered as the collection of all the periodic orbits plus the limiting orbits provided by the closure process. In this paper, we show that this assumption is to be taken with caution in a large class of scattering systems with at least three degrees of freedom. There exist more than one invariant sets, with different fractal dimensions, obtained in different constructions. Moreover, as far as the escape process is concerned, typical periodic orbits involving all the degrees of freedom of the system play a marginal role compared to the set generated by the gate.

This difference appears whenever the gate is a codimension one invariant subset in configuration space. A typical situation resulting in such subsets in scattering systems is the separation of one translational degree of freedom from internal degrees of freedom in the

asymptotic region. We will demonstrate this point in a simple planar three-body scattering problem describing the reactive collision of a single atom with a diatomic molecule. We explain our findings using this model as an illustrative example that we analyze from the point of view of treating general scattering processes.

II. A SIMPLE MODEL

A typical three-body scattering problem appearing in many contexts is a single particle interacting with a two-body system (usually integrable in itself); the most common examples are from chemical physics (reactive collisions) and celestial mechanics (planetary motion). Model problems of this type have been studied in several varieties, including ones restricted to two degrees of freedom. In fact, problems like reactive collisions in collinear or T-shape configurations [4,2] or the interaction of satellites in coplanar circular orbits (Hill's problem) [5] have become well-known representatives of chaotic scattering.

However, a more general treatment involving more than two degrees of freedom in these systems (and similar ones) is clearly necessary. We have chosen a planar atom-diatom collision with pairwise Morse potentials between the atoms at a total energy below the dissociation threshold so scattering consists of an exchange reaction. There are three qualitatively different channels corresponding to which of the three atoms escapes after the decay of the transient complex. Since we are more interested in the general topological properties of chaotic scattering rather than in accurate modelling of particular chemical reactions, we have chosen identical atomic masses and Morse potential parameters for simplicity.

In a center-of-mass coordinate system, the total number of degrees of freedom of this planar system is four, with total energy E and angular momentum J conserved. By choosing suitable new coordinates, the angle variable conjugate to J can be separated from the other three that still contain all the information on the relative distances of the atoms. For our purposes, the most appropriate choice is an abstract representation of the configuration by Cartesian coordinates (x, y, z) based on hyperspherical coordinates widely used for three-body problems [6–8].

The new variables and their time derivatives can then be used to express the kinetic energy K [7] and the interatomic distances r_{12}, r_{13} and r_{23} [8]. The actual expressions are rather complicated; we refer the interested reader to the literature on these coordinate systems, especially the references given above. The Hamiltonian takes the (dimensionless) form

$$H(x, y, z, p_x, p_y, p_z) = K + V_M(r_{12}) + V_M(r_{13}) + V_M(r_{23}) \tag{1}$$

where $V_M(r) = (1 - e^{-r})^2$ is the Morse potential. For simplicity, we confine ourselves to cases with $J = 0$. The explicit Hamiltonian and the equations of motion are given in Eqs. (60–66) of Ref. [7].

Important dynamical symmetries and special cases are reflected in these coordinates. The potential is mirror symmetric with respect to the plane $z = 0$ which corresponds to collinear configurations, and the plane $y = 0$ together with its two images obtained by rotation around the z axis by $\pm 2\pi/3$ contain symmetric T-shape configurations. For a given energy E below the total dissociation threshold $E_{\text{tot}} = 3$, the z variable is confined to a range

$[-z_{\max}, z_{\max}]$, while x and y can be arbitrarily large. The three channels corresponding to the three different outcomes of the reaction extend to infinity along the intersection lines of the T-shape planes with the collinear one. The boundaries of the three-dimensional energy surface, defined by $K = 0$, are plotted as usual surfaces in the abstract (x, y, z) space for a typical scattering energy in Fig. 1.

The escape channels of the scattering have asymptotically an axial symmetry as the distance from the origin tends to infinity. This is due to the separation of the translational motion of the outgoing single atom from the bound rotation/vibration of the molecule (a two-dimensional Morse oscillator). This observation will be of crucial importance concerning the topological properties of the system.

III. GATE OBJECTS IN HIGHER DIMENSIONS

For an object to act as a gate in a scattering process, it must have manifolds of codimension one in phase space. In general, time-independent Hamiltonian systems with n degrees of freedom can be represented in Poincaré sections of dimension $D = 2n-2$. Because of time reversal symmetry, hyperbolic orbits have stable and unstable manifolds of equal dimensionality: $d = n-1$. Thus a stable manifold of a hyperbolic periodic orbit is of codimension one in the Poincaré section for $n = 2$ only. Consequently, as soon as $n > 2$, the periodic orbits cannot anymore act as gates.

However, it has been pointed out by Wiggins [9] that in a three-dimensional configuration space, a two-dimensional invariant subset which is hyperbolic in the perpendicular direction have codimension one stable and unstable manifolds in the phase space of the three-degree-of-freedom system. Such objects can act as gates to a scattering process, provided their location in phase space makes it possible. In scattering systems like ours that can separate into a subsystem with $n - 1 = 2$ degrees of freedom plus 1 translational degree of freedom, such a $d = 2$ dimensional invariant object naturally exists: it consists of the lower-dimensional subsystem plus the outgoing particle standing infinitely far away from it. In fact, it has been shown by Toda [10] that in a planar atom-diatom collision the dynamics of the molecule and the third atom at rest defines an object in the four-dimensional Poincaré section with three-dimensional stable and unstable manifolds.

We show in the following that these manifolds define an invariant set for the scattering process that is superior in dimension to the set defined by the typical—i.e., three-body—periodic orbits. In this sense this larger set is the natural generalization of the usual chaotic invariant set of two-degree-of-freedom scattering systems.

IV. INVARIANT SETS AND THEIR DIMENSIONS

By definition, the intersection points of the stable and unstable manifolds of an invariant object define an invariant set for the dynamics. In our scattering model, the gate object in configuration space is a two-dimensional subset (an annulus) at the “end” of the outgoing channel. In the Poincaré section, the gate appears as a 2-d object too. In the remaining two dimensions in its vicinity, one can draw a curve from each point of the gate so that initial conditions on the curve will lead to asymptotic convergence to the orbit started from

the point on the gate. The stable manifold of the gate is then the collection of these curves forming locally a three-dimensional object.

Because of the global stretching and folding generated by the nonlinear dynamics of the system, this manifold also has a fractal structure in the direction perpendicular to it, so globally it has a total dimension $d_g = 3 + \delta$ with $0 < \delta < 1$ being the partial fractal dimension in the perpendicular direction. Because of time reversal symmetry, the unstable manifold must have the same dimension. Their intersections define an invariant set with a dimension

$$d_{sg} = 2d_g - D = 2 + 2\delta, \tag{2}$$

where $D = 4$ is the dimension of the Poincaré section (the embedding dimension), and the subscript "sg" indicates the invariant *set* generated by the *gate*. In contrast, if we consider an inner periodic orbit (i.e. one which is not part of the gate) with locally 2-d stable and unstable manifolds that have fractal properties in two other directions characterized by partial fractal dimensions ϵ_1 and ϵ_2, then the invariant set defined by these $d_p = 2 + \epsilon_1 + \epsilon_2$ dimensional manifolds have a total dimension

$$d_{sp} = 2d_p - D = 2(\epsilon_1 + \epsilon_2). \tag{3}$$

In order to compare the dimensionalities of these two different invariant sets, we first consider the partial dimensions δ, ϵ_1 and ϵ_2 of the invariant manifolds. Since the stable manifolds of two different objects cannot cross, the 2-d branches of stable manifolds of periodic orbits must run locally parallel to one another and, in particular, along the 3-d branches of the stable manifold of the gate object. Moreover, they are on one side of the stable gate manifold. This is because if a trajectory is to approach a certain periodic orbit from a given initial point in phase space, then it must avoid escape until it reaches the vicinity of the periodic orbit. This can happen only if the starting point is on the "right" side of the 3-d stable branch of the gate. Therefore the stable branch of the periodic orbit going through that point must follow the foldings of the gate manifold, so one of the two directions along which the periodic orbit manifolds show fractality must coincide locally with the fractal direction of the gate manifold. This implies that the corresponding partial fractal dimension—say, ϵ_1—is equal to δ. The spatial relationship of the gate manifolds and those of the inner periodic orbits is illustrated schematically in Fig. 2.

As an immediate consequence, we obtain that $d_{sg} > d_{sp}$, i.e., the invariant set generated by the gate manifolds is of higher dimension than the invariant set belonging to the inner periodic orbits. In other words, we have a situation where the inner periodic orbits are nowhere dense in the set of nonescaping orbits. This is in sharp contrast to two-degree-of-freedom open Hamiltonian systems, where the inner periodic orbits are everywhere dense in the invariant phase space sets. Our example demonstrates that the denseness of periodic orbits in invariant sets of higher dimensional systems cannot be taken for granted without further considerations. In our case, without the periodic orbits of the gate itself, considered "trivial" from the point of view of the full dynamics of the system, there is no dense set of periodic orbits for the larger invariant set.

V. STABLE AND UNSTABLE MANIFOLDS IN THE TRIPLE MORSE-SYSTEM

Following the approach of Chen et al. (Ref. [11]), we can represent the stable and unstable manifolds and the invariant sets on planar (2-d) sections of the four-dimensional phase space. For this purpose, we chose initial conditions on the Poincaré section with two fixed restrictions and two free parameters. In this paper, the Poincaré section is defined by $y = 0$ (with $v_y > 0$) while the particular restrictions in the initial conditions are $x_0 + z_0 = 0$ and $v_{0x} + v_{0z} = 0$. We plotted each initial point on the (z_0, v_{0z}) plane by using a colour coding according to the exit channel the trajectory starting from that point eventually took; the result is shown in Fig. 3.

It is clear from this picture that all three colours form compact regions with smooth boundaries. The boundary of a single-coloured region consists of trajectories with vanishing translational kinetic energy at the "end" of the channel, i.e., those asymptotic to the corresponding gate object. In other words, the smooth curves obtained as the boundaries of regions of a given colour are just the planar sections of the stable manifold of the gate closing the channel associated with that colour. On the outer side of these curves, smaller, differently coloured regions can be found, accumulating on the boundaries in a fractal manner. Similar pictures have been presented in Ref. [12] for the gravitational three-body problem.

In fact, the stable manifold curves of Fig. 3 are an example of Wada boundaries [13], i.e. fractal boundary sets where all three colours are present in any neighbourhood of the boundary. It is worth noting that in chaotic scattering processes with more than two distinct possibilities for the outgoing motion, Wada boundaries are typical [14], but such objects can also appear, e.g., as physical boundaries between dyes of different colour poured into open hydrodynamical flows [15].

In order to obtain the planar sections of the unstable manifolds of the gate objects, one should follow the trajectories from the same initial conditions backward in time. However, our initial conditions lie in a symmetry plane of the potential (T-shape configurations), so following a trajectory backward from an initial condition (z_0, v_{0z}) is equivalent to following the forward-time trajectory starting from the point $(z_0, -v_{0z})$. Thus the unstable manifold curves in our planar section can be obtained by mirroring the stable manifold curves with respect to the z_0 axis in Fig. 3.

The sets of stable and unstable manifold curves cross each other, and the crossing points form the planar section of the invariant set associated with the gates. In the case of Fig. 3, we can plot an approximation of the cross section points by considering a colour pixel as a cross section point if both itself and its mirror image on the other side of the z_0 axis have at least one neighbour cell of different color. The result is shown on Fig. 4; the fractal nature of the plot is indicated by a blowup. According to the considerations of the dimensions in the previous section, each point in this plot represents a smooth two-dimensional object in the total invariant set embedded in the four-dimensional phase space of the Poincaré map. In other words, our plot captures the fractal part of the invariant set associated with the gate, having a fractal dimension of 2δ.

It is important to stress that since the crossing of two 2-d objects in a 4-d space is generic, we can expect that a similar plot of the gate invariant set can be obtained in all similar systems with any value of δ. On the other hand, the invariant set associated with the inner periodic orbits may or may not produce points in a planar section depending on

whether $\epsilon_1 + \epsilon_2$ is larger or smaller than 1; see the discussion of this aspect in Ref. [11].

VI. LINEAR SECTIONS AND SCALING PROPERTIES

One of the convenient characteristics of two-degree-of-freedom chaotic scattering is that its scaling properties can be studied through one-dimensional sets of initial conditions. However, as has been shown in Ref. [11], this property may or may not be true in general hyperbolic chaotic scattering with 3 degrees of freedom, depending on the value of the fractal dimension of the invariant set and its stable manifold. In this paper, we have shown evidence that in three-degree-of-freedom scattering systems with the asymptotic separation of one degree of freedom, the feasibility of the one-dimensional description is restored. The reason for this is that in such systems the crossing of the 3-d stable manifolds with a line in the 4-d phase space is a generic property. This means that typically any 1-d family of initial conditions would lead to scattering functions with a fractal set of singularities, as in two-degree-of-freedom chaotic scattering. These singularities are the fingerprints of the fractal structure of the stable manifold of the gate.

To check this point, we have produced plots of the scattering time for various linear sets of initial conditions in our triple Morse model. They all showed the typical singular behaviour well known from two-degree-of-freedom chaotic scattering examples. We also analyzed the singularities to determine the *uncertainty exponent* α_u, which is related to the (partial) fractal dimension as $\delta = 1 - \alpha_u$ [16]. The uncertainty exponent can be measured by choosing pairs of initial conditions with a separation of ε along the line: the rate $p(\varepsilon)$ of pairs where the two orbits escape along different channels scales as $p(\varepsilon) \sim \varepsilon^{\alpha_u}$. We have obtained a value of 0.12 for α_u, which gives a fractal dimension $\delta = 0.88$ for the stable manifold of the gates.

It is worth noting that although we measured the fractal dimension of the stable manifold of the gates, this scaling behaviour cannot originate from the gates themselves since they are only marginally unstable due to the behaviour of the Morse potential: The marginal instability of the gates should lead to an asymptotic fractal dimension value of 1. However, if our statistics is based on moderately long scattering orbits, we can still observe a scaling region associated with an apparent fractal dimension which is lower than 1 as if there were only hyperbolic orbits in the system. In our model, the only truly hyperbolic orbits are the inner periodic orbits, so the observed scaling can only be produced by them. This indicates that although these orbits form an invariant set inferior in dimension to the invariant set of the gate, they can still dictate the fractal scaling properties, based on moderately long orbits, of the larger invariant set.

VII. CONCLUSIONS

We have shown in the example of a simple model that for a large class of three-degree-of-freedom chaotic scattering systems, the asymptotic separation of a translational degree of freedom leads to a gate object regulating the escape process, and that the gate itself then defines an invariant set of larger dimension than the one generated by the hyperbolic inner periodic orbits. In fact, although the invariant set associated with these periodic orbits is

part of the invariant set associated with the gate, the inner periodic orbits are nowhere dense in the larger invariant set of the gate. The usual assumption that periodic orbits are dense in an invariant set is valid in these cases only if we consider also the periodic orbits in the gate, although they, as "trivial" ones, are not readily associated with the "true" three-body dynamics of the system. Actually, most of the points of the larger invariant set are either periodic orbits of the gate or asymptotic to them, leaving zero measure to scattering trajectories asymptotic to inner periodic orbits.

We have also demonstrated, however, that the inner periodic orbits can still determine the scaling properties of the larger invariant set due to the fact that their manifolds run locally alongside the manifolds of the gate object. This leaves open the question concerning which sets of periodic orbits are to be taken into account in descriptions based on periodic orbit theory in larger dimensional systems: in general, we cannot exclude the existence of cases when the gate periodic orbits have dominating contributions to sums involving all periodic orbits of the system.

Although we treated only one example in three-degree-of-freedom chaotic scattering, our findings can be generalized to any Hamiltonian problem described by a four-dimensional Poincaré map with a suitable two-dimensional invariant subspace. Another possible way of extension can be considering systems with more than 3 degrees of freedom: if there is an asymptotic separation of only one degree of freedom from the rest, then in principle gate objects can be defined in an analogous way, and the topological consequences can be similar too. An obvious example is the full spatial dynamics of a three-body collision that can be reduced to four nontrivial degrees of freedom.

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FIGURES

FIG. 1. $K = 0$ surfaces in the abstract representation for $E = 2.4$. Because of the mirror symmetry of the potential, only the $z \geq 0$ halves are shown. The trajectories must stay in the domain between the red and green surfaces. The $z = 0$ contours on the base are the $K = 0$ curves for collinear configurations. The labels next to the exit channels give the colour coding used in Fig. 3 for the outcome of the scattering process.

FIG. 2. Schematic picture of the stable manifold of the gate object and those of the inner periodic orbits. In a two-dimensional slice of the four-dimensional phase space, the 2-d stable manifolds of periodic orbits appear as dots forming a double Cantor set structure. The 3-d stable manifold of the gate object appears in the same section as a continuous line folded by the dynamics so that it has fractal structure in one direction. The partial fractal dimension δ of the folded line agrees with the partial fractal dimension ϵ_1 of the double Cantor set along the same direction. This picture also indicates that in the vicinity of a periodic orbit manifold, one can always find points from the stable manifold of the gate, while the opposite is not true. The binary organization of the Cantor set and the folding structure is chosen only for simplicity.

FIG. 3. Initial conditions from the 2-d subspace of the Poincaré section coloured according to the exit channel of the corresponding trajectory. The boundary curves of the single-colour regions are the slices of the stable manifold of the gate object.

FIG. 4. Approximation of the planar cross section of the invariant set defined by the gate manifolds (a). The picture shows the signs of a fractal structure indicated by the blowup (b) of a small region that looks homogeneous on a lower resolution.

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